Crystal structure of 4,6-dinitro-1-(5-tetrazolyl)-1H-indazole trihydrate

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Abstract

The title compound, \( \text{C}_8\text{H}_4\text{N}_8\text{O}_4 \cdot 3\text{H}_2\text{O} \), crystallizes in space group \( P\bar{1} \) with cell constants \( a = 7.022(1), b = 9.507(2), c = 10.906(2) \text{ Å}, \alpha = 84.99(1), \beta = 71.89(1), \gamma = 72.56(1)^\circ, Z = 2, \) and \( V_c = 660.2 \text{ Å}^3 \). The structure was solved by direct methods using diffractometer data and was refined by full-matrix least-squares methods to an \( R \) value of 0.060 for 2112 observed reflections. The molecule, consisting of a phenyl ring fused to a pyrazole ring with a tetrazole ring connected to it equatorially, is planar except for the \( N(7) \) nitro-group oxygen atoms. The structure is stabilized by a three-dimensional network of \( \text{O} - \text{H} \cdots \text{O}, \text{O} - \text{H} \cdots \text{N}, \) and \( \text{N} - \text{H} \cdots \text{O} \) hydrogen bonds through the water molecules.

Introduction

The compound 2,4,6-trinitrobenzaldehyde-1\( H(2H) \)-tetrazol-5-yl-hydrazone used in the preparation of explosives, is obtained by the reaction of 5-hydrazinotetrazole hydrochloride in aqueous solution with 2,4,6-trinitrobenzaldehyde in alcohol (Om Reddy \textit{et al.}, 1981) and is usually recrystallized from dimethyl formamide solution. The structure proposed on the basis of analytical studies using UV, IR, NMR, and mass spectrophotometric
techniques is shown in Fig. 1a. Thermal studies on several tetrazole derivatives using a differential scanning calorimeter have indicated that the reactivity of these compounds increases with increasing number of nitro groups in the phenyl ring (Om Reddy et al., 1981). However, the structure obtained during this crystal structure analysis using single crystal X-ray diffraction revealed the absence of one of the nitro groups, the presence of